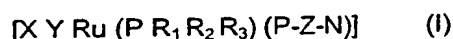


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Claims:

1. Process for hydrogenating a substrate containing a carbon-heteroatom double bond, which includes the step of reacting the substrate with hydrogen in the presence of a hydrogenation catalyst and of a base, characterized in that the hydrogenation catalyst is a transition metal complex of the formula (I)

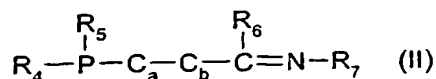


where

X, Y are each independently a hydrogen atom, halogen atom, C<sub>1-8</sub>alkoxy or C<sub>1-8</sub>acyloxy group, or a coordinatively bound organic solvent molecule containing at least one heteroatom having at least one free electron pair, for example in the form of (cyclo)alkyl/aryloxy, -thio or -amino groups, in which case the charge of the resulting cationic complex is balanced by an anion, for example CN<sup>-</sup>, OCN<sup>-</sup>, PF<sub>6</sub><sup>-</sup> or F<sub>3</sub>C-SO<sub>2</sub>O<sup>-</sup>,

R<sub>1</sub>, R<sub>2</sub>, R<sub>3</sub> are each independently an alkyl, alkyloxy, alkylthio, dialkylamino, cycloalkyl, cycloalkyloxy, cycloalkylthio, dicycloalkylamino, aryl, aryloxy, arylthio or diarylamino group, optionally substituted by 1, 2 or 3 radicals which are each independently selected from C<sub>1-4</sub>alkyl groups and C<sub>1-4</sub>alkoxy groups, or one of the R<sub>1</sub>, R<sub>2</sub>, R<sub>3</sub> radicals is as defined above and the remaining 2 radicals which, linked either via an oxygen bridge or directly to the phosphorus atom, form, including the phosphorus atom, a 4- to 8-membered, optionally substituted ring,

P-Z-N is a bidentate ligand which contains an sp<sup>2</sup>-hybridized nitrogen atom and is of the formula (II)



where

R<sub>4</sub>, R<sub>5</sub> are each independently a linear, branched or cyclic C<sub>1-8</sub>alkyl or C<sub>2-8</sub>alkenyl group, optionally substituted; C<sub>6-18</sub>aryl, C<sub>3-18</sub>heteroaryl, C<sub>3-8</sub>cycloalkyl, (C<sub>1-8</sub>Alkyl)<sub>1-3</sub>-(Hetero)Aryl, optionally substituted, whereby possible substituents are halogen, organohalogen group, O(C<sub>1-8</sub>)alkyl, N(C<sub>1-8</sub>alkyl)<sub>2</sub>; or R<sub>4</sub> and R<sub>5</sub> together are a saturated or aromatic ring composed of 5 to 10 atoms including the phosphorus atom,

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C<sub>a</sub>, C<sub>b</sub> are each a part of an aromatic, optionally substituted (hetero)aryl having at least 6  $\pi$ -electrons,

R<sub>6</sub> is a hydrogen atom, a linear, branched or cyclic C<sub>1-10</sub>alkyl or C<sub>2-10</sub>alkenyl group, optionally substituted, an aromatic ring, optionally substituted, a -OR<sub>6</sub> or -NR<sub>6</sub>R<sub>6</sub> radical, where R<sub>6</sub> and R<sub>6</sub><sup>-</sup> are as defined for R<sub>6</sub>,

R<sub>7</sub> is a hydrogen atom, a linear, branched or cyclic C<sub>1-10</sub>alkyl or C<sub>2-10</sub>alkenyl group, or an R<sub>7</sub>CO or R<sub>7</sub>SO<sub>2</sub> radical where R<sub>7</sub> is a C<sub>1-8</sub>alkyl or aryl group,  
or

R<sub>6</sub> and R<sub>7</sub> together are an unsaturated (hetero)cycle composed of 5 to 10, optionally substituted ring atoms, including the carbon and the nitrogen atom to which R<sub>6</sub> and R<sub>7</sub> are bonded, and optionally including further heteroatoms.

2. Process according to Claim 1, characterized in that X, Y in the formula (I) are each independently a hydrogen atom or a halogen atom.

3. Process according to Claim 2, characterized in that X, Y in the formula (I) are each a halogen atom, in particular chlorine.

4. Process according to one of Claims 1 to 3, characterized in that R<sub>1</sub>, R<sub>2</sub>, R<sub>3</sub> in the formula (I) are each independently a methyl, ethyl, propyl, i-propyl, n-butyl, i-butyl, sec-butyl, tert-butyl, cyclopentyl, cyclohexyl, phenyl, o- or p-tolyl, p-isopropylphenyl or mesityl group.

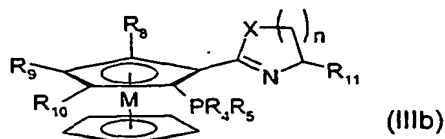
5. Process according to one of Claims 1 to 4, characterized in that R<sub>4</sub>, R<sub>5</sub> in the formula (I) are each independently a radical selected from methyl, ethyl, n-propyl, i-propyl, n-butyl, i-butyl, cyclohexyl, phenyl, o- or p-tolyl, mesityl,  $\alpha$ - or  $\beta$ -naphthyl.

6. Process according to one of Claims 1 to 5, characterized in that C<sub>a</sub>, C<sub>b</sub> in the formula (II) are part of a pure 6  $\pi$ -electron system in the form of optionally substituted benzene or in the form of an optionally substituted cyclopentadienide ion as a ligand of a metallocene.

7. Process according to one of Claims 1 to 6, characterized in that R<sub>6</sub> and R<sub>7</sub> in the formula (II) together are an unsaturated heterocycle composed of 5 to 10, optionally substituted ring atoms, including the carbon and the nitrogen atom to which R<sub>6</sub> and R<sub>7</sub> are bonded, and optionally including further heteroatoms.

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8. Process according to one of Claims 1 to 5, characterized in that the ligand of the formula (II) is a ligand of the general formula (IIIb)



where

$n = 1$  or  $2$ , preferably  $1$ ,

$M = \text{Fe, Ru, Os}$ , preferably  $\text{Fe}$ ,

$X = \text{O, S or N}$ , preferably  $\text{O}$ ,

$R_4, R_5$  are each radicals corresponding to the definition given under formula (II),

$R_{11}$  is a  $\text{C}_{2-8}$ alkoxyalkyl,  $\text{C}_{7-19}$ aralkyl,  $\text{C}_{3-18}$ heteroaryl,  $\text{C}_{4-19}$ heteroaralkyl,

$(\text{C}_{1-8}\text{alkyl})_{1-3}\text{-C}_{6-18}(\text{hetero})\text{aryl}$ ,  $(\text{C}_{1-8}\text{alkyl})_{1-3}\text{-C}_{6-18}\text{cycloalkyl}$ ,  $\text{C}_{3-8}\text{cycloalkyl}$ ,

$\text{C}_{3-8}\text{cycloalkyl-C}_{1-8}\text{alkyl radical}$ , or preferably  $\text{C}_{1-6}\text{alkyl}$ ,  $\text{C}_{6-18}\text{aryl radical}$ , in particular  $i\text{-propyl}$ ,

and the radicals mentioned may be substituted by one or more heteroatoms such as  $\text{Hal, Si, N, O, P, S}$ , or the radicals may have one or more heteroatoms such as  $\text{Si, N, O, P, S}$  in their carbon framework,

$R_{8,9,10}$  are each independently a  $\text{C}_{1-8}\text{alkyl}$ ,  $\text{C}_{2-8}\text{alkoxyalkyl}$ ,  $\text{C}_{6-18}\text{aryl}$ ,  $\text{C}_{7-19}\text{aralkyl}$ ,

$\text{C}_{3-18}\text{heteroaryl}$ ,  $\text{C}_{4-19}\text{heteroaralkyl}$ ,  $(\text{C}_{1-8}\text{alkyl})_{1-3}\text{-C}_{6-18}(\text{hetero})\text{aryl}$ ,  $\text{C}_{3-8}\text{cycloalkyl}$ ,

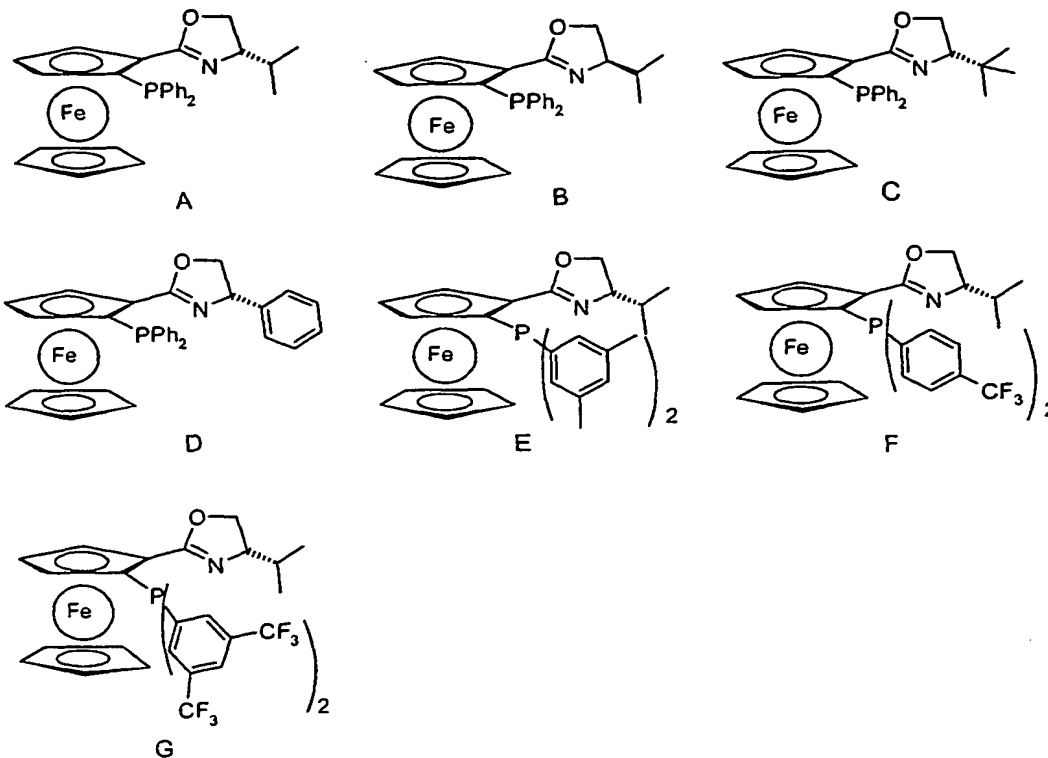
$(\text{C}_{1-8}\text{alkyl})_{1-3}\text{-C}_{6-18}\text{cycloalkyl}$ ,  $\text{C}_{3-8}\text{cycloalkyl-C}_{1-8}\text{alkyl radical}$ , or preferably  $\text{H}$ , and the radicals

mentioned may be substituted by one or more heteroatoms such as  $\text{Hal, Si, N, O, P, S}$ , or

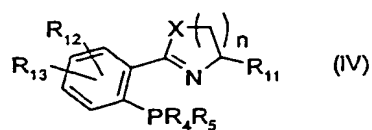
the radicals may have one or more heteroatoms such as  $\text{Si, N, O, P, S}$  in their carbon framework.

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9. Process according to Claim 8, characterized in that the ligand of the formula (IIIb) is selected from the ligands A to G:



10. Process according to one of Claims 1 to 5, characterized in that the ligand of the formula (II) is a ligand of the general formula (IV)



where

$n = 1$  or  $2$ , preferably  $1$ ,

$X = O, S$  or  $N$ , preferably  $O$ ,

$R_4, R_5$  are each radicals corresponding to the definition given under formula (II),

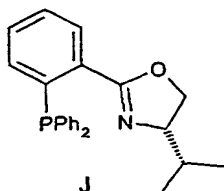
$R_{11}$  is a  $C_{2-8}$ alkoxyalkyl,  $C_{7-19}$ aralkyl,  $C_{3-18}$ heteroaryl,  $C_{4-19}$ heteroaralkyl,  $(C_{1-8}alkyl)_{1-3}-C_{6-18}(hetero)aryl$ ,  $(C_{1-8}alkyl)_{1-3}-C_{6-18}cycloalkyl$ ,  $C_{3-8}cycloalkyl$ ,

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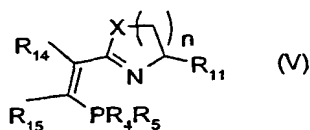
C<sub>3-8</sub>cycloalkyl-C<sub>1-8</sub>alkyl radical, or preferably C<sub>1-8</sub>alkyl, C<sub>6-18</sub>aryl radical, in particular i-propyl, and the radicals mentioned may be substituted by one or more heteroatoms such as Hal, Si, N, O, P, S, or the radicals may have one or more heteroatoms such as Si, N, O, P, S in their carbon framework,

R<sub>12</sub>, R<sub>13</sub> are each independently a C<sub>1-8</sub>alkyl, C<sub>1-4</sub>alkoxy radical, or preferably H, or are together a fused cycloalkyl or aryl ring.

12. Process according to Claim 11, characterized in that the ligand of the formula (IV) corresponds to the formula J:



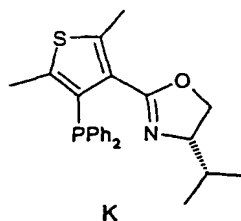
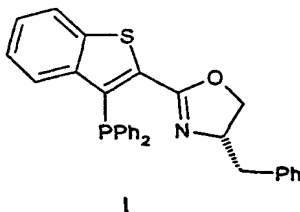
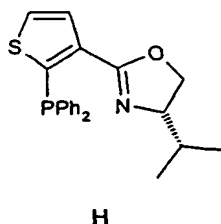
13. Process according to one of Claims 1 to 5, characterized in that the ligand of the formula (II) is a ligand of the general formula (V)



where

n, X, R<sub>4</sub>, R<sub>5</sub> and R<sub>11</sub> are each as defined in Claim 10 for formula (IV), and R<sub>14</sub> and R<sub>15</sub> together are a 6  $\pi$ - or 10  $\pi$ -electron heteroaromatic system, optionally substituted by linear or branched C<sub>1-8</sub>alkyl radicals, and possible heteroatoms are N, O, or S.

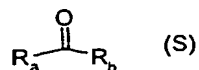
14. Process according to Claim 13, characterized in that the ligand of the formula (V) corresponds to one of the formulae H, I and K:



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15. Process according to Claim 1, characterized in that the substrate to be hydrogenated is a prochiral imine or ketone.

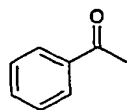
16. Process according to Claim 15, characterized in that the substrate to be hydrogenated is a prochiral ketone of the general formula (S)



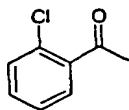
where  $\text{R}_a$  and  $\text{R}_b$  are each independently a hydrogen atom, a cyclic, linear or branched  $\text{C}_{1-8}$ alkyl or  $\text{C}_{2-8}$ alkenyl group, or an monocyclic or polycyclic aryl or heteroaryl group, optionally substituted by linear or branched  $\text{C}_{1-8}$ alkyl,  $\text{C}_{1-8}$ alkoxy groups, or halogen atoms.

17. Process according to Claim 16, characterized in that the substrate to be hydrogenated is a prochiral monocyclic or polycyclic aryl ketone or heteroaryl ketone, optionally substituted by linear or branched  $\text{C}_{1-8}$ alkyl,  $\text{C}_{1-8}$ alkoxy groups, or halogen atoms.

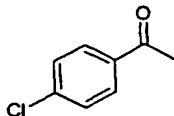
18. Process according to Claim 17, characterized in that the substrate to be hydrogenated is selected from one of ketones 1 to 7:



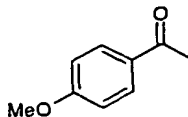
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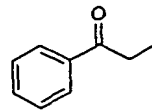
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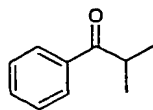
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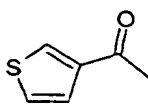
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